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Massively Parallel Constrained Force Algorithm for MD Simulation of Polymers and Dendrimers AMIR FIJANY, *JPL, Caltech*, TAHIR CAGIN, *MSC, Caltech*, ANDRES JARAMILLO-BOTERO, *MSC, Caltech*, SANDEEP GULATI, *JPL, Caltech*, WILLIAM A. GODDARD, III, **MSC, Caltech** — We have recently developed the Parallel Constraint Force Algorithm for systems with a serial chain topology, resulting in a both time- and processor-optimal solution of Equations of Motion, This is an $O(Log\,N)$ algorithm by using $O(N)$ processors. The **CF** algorithm is also highly efficient for practical implementation on massively parallel MIMD architectures due to its coarse grain size and simple communication structure. We will discuss the application of the **CF** algorithm to large scale MD simulations of systems with serial chain topology, Polyethylene (**PE**). We show that with $P < N$ processors, the CF algorithm is optimally implemented with a cost of $O(N/P + Log\,P)$. Many applications of interest involve systems with more complex topologies, such as branched, grafted polymers and **hyperbranched, dendrimers.** We also present a more efficient variant of the CF algorithm for systems with such topologies. For example, considering a branched topology system with N rigid bodies, each having one or more branches with L bodies, this variant of the CF algorithm achieves an optimal computation time of $O(Log\,N + P)$ by using $O(N)$ processors.

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